Review of EPA Region VIII Draft Report: "Dispersion Modeling Analysis of PSD Class I Increment Consumption in North Dakota and Eastern Montana"

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1.0 INTRODUCTION

In 1999, the North Dakota Department of Health (NDDH) conducted a draft modeling study that showed potential increases of SO_2 concentrations in four Prevention of Significant Deterioration (PSD) Class I areas in western North Dakota. These increases were predicted to be higher than the incremental degradation allowed under the provisions of the Clean Air Act amendments of 1977. In March 2001, the NDDH made a commitment to the United States Environmental Protection Agency (EPA) Region VIII to refine the modeling approach and to adopt any necessary revisions to the State Implementation Plan (SIP) to address any modeled violations of the PSD increment.

In March 2002, the EPA released their own version, dated January 2002, of a refined modeling approach that still indicates potential violations of the 3-hour and 24-hour SO_2 PSD increments. EPA is asking for public comments on all aspects of the modeling analysis. Elements of the analysis discussed in this report include the following:

- Regulatory status and limitations of the CALPUFF modeling system used in the EPA analysis (see Section 2),
- The limited evaluation study of CALPUFF conducted by the NDDH and relied upon by the EPA (see Section 3), and
- Other aspects of the modeling analysis, including the PSD emission inventory and SO_2 monitoring trends (see Section 4).

Conclusions are presented in Section 5, and References are provided in Section 6.

2.0 CALPUFF/CALMET MODELING SYSTEM

2.1 CALPUFF AS A PROPOSED EPA GUIDELINE MODEL

CALPUFF (Scire et al., 2000) has been formally proposed by the United States Environmental Protection Agency (EPA) as a guideline model for assessing long-range transport impacts (that is, covering distances of over 50 kilometers). There have been a number of public comments on the CALPUFF modeling procedures, including limitations in the model's range of applicability and tendency to over predict at large distances (beyond 100 kilometers). EPA has not yet released a final version of the model in response to these comments, although a "beta test" version for review and comment was released in the fall of 2001. Until the model is finalized for promulgation, any applications with current versions of CALPUFF need to be considered as preliminary and subject to change.

To get to this point, the EPA and the Federal Land Managers (FLMs) formed an Interagency Workgroup on Air Quality Modeling (IWAQM) in the early 1990s to produce a consistent approach to assessing impacts in Federal Class I Areas. The IWAQM plan of model development involved a phased approach. Phase 1 consisted of reviewing EPA guidance and recommending an interim modeling approach to meet the immediate need for a long-range transport model for ongoing permitting activity. In developing a Phase 2 recommendation, the IWAQM workgroup reviewed other available operational models and made a recommendation of the most appropriate modeling techniques.

Given the practical limitations of resources and hardware, the IWAQM Phase 1 interim recommendations (U.S. EPA, 1993) were designed to provide the best approach from existing "off-the-shelf" techniques. Two candidate models were assessed, the MESOPUFF II model (U.S. EPA, 1994) and the Acid Rain Mountain Mesoscale Model (ARM3), Morris, et al. (1988). Upon careful examination of both models, IWAQM discovered coding errors in the ARM3, which potentially invalidated its previous evaluations. With this in mind and other considerations as discussed in U.S. EPA (1993), IWAQM's Phase 1 recommendation was to use on a case-by-case basis the Lagrangian puff model, MESOPUFF II, to evaluate the impacts of pollutants from sources located more than 50 kilometers and up to several hundred kilometers from Class I areas. North Dakota faced the need to recommend such a model in the early 1980's, more than 10 years before the existence of IWAQM. It is noteworthy that the state of North Dakota was well ahead of IWAQM, having adopted the same model, MESOPUFF, to be used for assessing PSD Class I impacts in North Dakota.

For the Phase 1 IWAQM recommendation, MESOPUFF II was deemed suitable for conducting single source impact analyses, and in some circumstances cumulative impact analyses. Since the dispersion characterizations in MESOPUFF II were not designed to handle local-scale dispersion effects, it was recognized that the MESOPUFF II results would frequently need to be combined with the results from other modeling techniques used to estimate concentrations from sources closer than 50 kilometers to a receptor area. The Phase 1 recommendation was structured to satisfy case-by-case EPA modeling guideline criteria for cases where there is no preferred model, which was the case for long-range transport applications.

By restricting the models considered for Phase 1 to "off-the-shelf" techniques, IWAQM recognized certain limitations. These included a lack of consideration of the effects of terrain on the long-range transport and dispersion (MESOPUFF II does not consider terrain effects), an underestimation of the conversion of sulfur dioxide to sulfate when polluted air interacts with clouds, and a possible overestimation of particulate nitrate when a limited number of sources are considered. Nonetheless, IWAQM considered the techniques to be a significant improvement to those previously used, in that previous techniques ignored many of the processes important to the assessment of air quality impacts in Class I areas.

Not long after the release of the Phase 1 recommendation, the EPA sponsored the Sixth Modeling Conference, which was held August 9-10, 1995 in Washington, D.C. One of the main topics at this two-day event was a review of the IWAQM Phase 1 recommendation and a summary of work in progress, with review comments provided by several groups. At the conference, IWAQM presented long-range trajectory comparison that suggested that use of mesoscale meteorological analyses of wind fields provided a significant improvement in the modeling of modeled and observed trajectories. The IWAQM endorsed specifically the use of mesoscale meteorological analyses that employ data assimilation, such as the use of MM4 data (Anthes et al., 1987). The IWAQM recommended that the Phase 1 procedure to use the MESOPUFF II modeling system should be replaced with a Phase 2 recommendation to use the CALMET/CALPUFF modeling system. This Phase 2 model was a relatively new Lagrangian puff modeling system, which had additional algorithms to provide simulation of local-scale short-range dispersion using methods already endorsed by the EPA. Thus, use of this newer modeling system could allow one model to be used for all sources in an analysis, regardless of the transport distance involved. Significant improvements afforded by CALPUFF over MESOPUFF II were improved terrain handling, more vertical resolution in the wind field definition, and better handling of plume chemistry.

As a result of the IWAQM recommendation, EPA has proposed CALPUFF as a model to be used for long-range transport applications (with source-receptor distances beyond 50 kilometers). EPA also proposes that CALPUFF be considered on a case-by-case basis for short-range applications involving "complex winds", i.e., where straight-line steady-state plume transport models would not likely work very well. In the present North Dakota application that involves SO_2 impacts at the PSD Class I areas, most of the sources being modeled are in excess of 50 kilometers away. However, several of the oil and gas producing sources are within 50 kilometers. According to current and even future guidance, these sources may need to be run with the ISCST3 model, because the terrain involved is not so severe so as to make ISCST3 applications invalid. However, if the ISCST3 model does not properly credit emissions from increment expanding sources in complex terrain due to internal coding procedures to limit that credit, these sources should either be modeled with CALPUFF or the ISCST3 modeling should be done separately for increment consuming and expanding sources and the results added in a postprocessor.

EPA proposed the use of CALPUFF as a guideline model for long-range transport applications in a *Federal Register* notice on April 21, 2000. There was a subsequent comment period that ended in August, 2000. To date, model improvements such as the inclusion of the PRIME downwash algorithm have not been installed into CALPUFF. It is unclear what the final version of CALPUFF will look like prior to release in the EPA promulgation package. Therefore, use of the current version of CALPUFF is subject to change.

2.2 Limitations of CALPUFF

Although EPA is on a path to promulgate CALPUFF as a guideline model for long-range transport applications, there are a number of remaining implementation issues and model limitations. Generating wind fields with CALMET using multiple sites for surface and upper air data introduces a number of technical challenges for the model user.

Although many technical model options have default selections, site-specific considerations are often necessary, and there is relatively little guidance available on the considerations that need to be taken into account in making these selections. The North Dakota Department of Health (NDDH) has done an extensive review of the model options for the CALPUFF modeling of impacts at PSD Class I areas in the state.

A limited number of evaluations of CALPUFF has been completed by the U. S. EPA. The following summary information is provided in Section 2.3.2 and in Appendix D of the IWAQM Phase 2 Summary Report. It indicates distance and time travel limitations regarding CALPUFF applications.

From Section 2.3.2 of the IWAQM Phase 2 report:

> *"...it appears that CALPUFF provides reasonable correspondence with observations for transport distances of order 100 km. Most of these comparisons involved concentration values averaged over 5 to 12 hours. The CAPTEX comparisons, which involved comparisons at receptors that were 300 km to 1000 km from the release, suggest that CALPUFF tends to overestimate surface concentrations by a factor of 3 to 4. Use of the puff splitting option in CALPUFF might have improved these comparisons, but there are serious conceptual concerns with the use of puff dispersion at very long-range transport (300 km and beyond). As the puffs enlarge due to dispersion, it becomes problematic to characterize the transport by a single wind vector, as significant wind direction shear may well exist over the puff dimensions."*

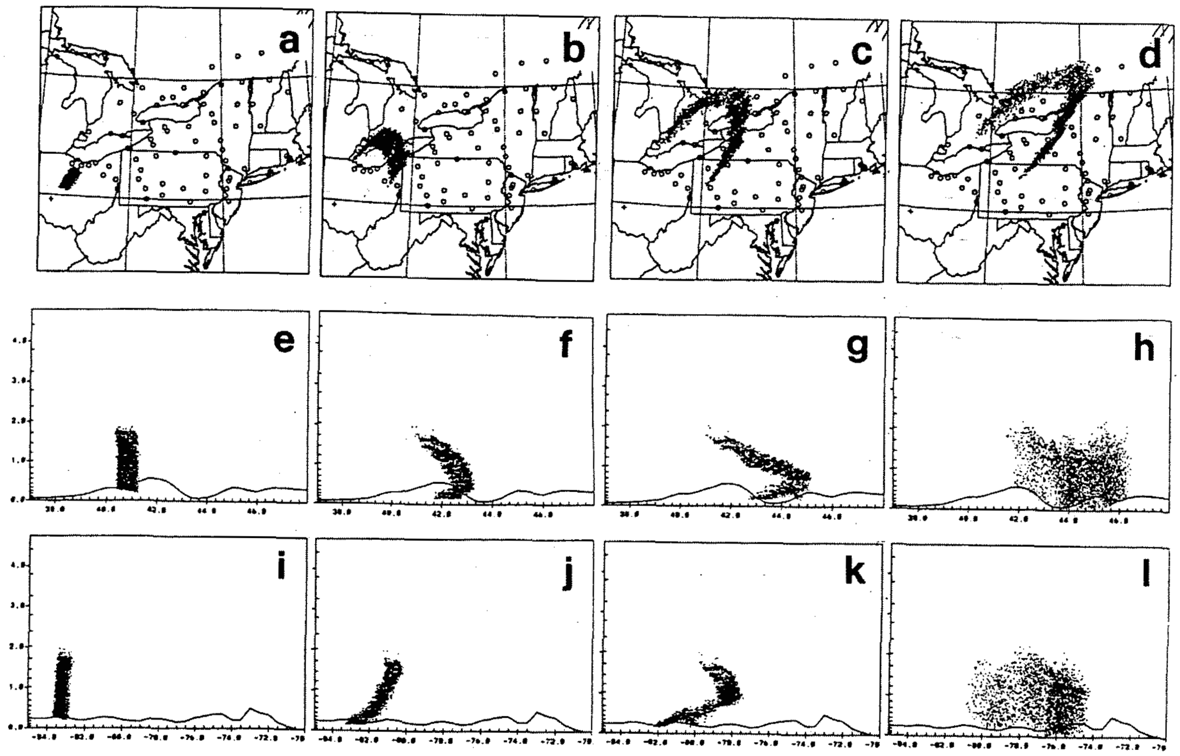
From Appendix D of the IWAQM Phase 2 report:

> *"...The IWAQM concludes that CALPUFF can be recommended as providing unbiased estimates of concentration impacts for transport distances of order 200 km or less, and for transport times of order 12 hours or less. For larger transport times and distances, our experience thus far is that CALPUFF tends to underestimate the horizontal extent of the dispersion and hence tends to overestimate the surface-level concentration maxima. This does not preclude the use of CALPUFF for transport beyond 300 km, but it does suggest that results in such instances be used cautiously and with some understanding."*

It would appear from the above IWAQM findings that at a distance of 200 kilometers, the CALPUFF modeling estimates would be likely to have an over prediction tendency somewhere between the unbiased ratio of 1 at 100 km and the ratio of 3 to 4 at 300 km and beyond. An overprediction tendency at a distance of 200 kilometers of about 2 may be expected. This expectation is explored further in Section 3 with the analysis of the NDDH evaluation of CALPUFF using data from the year 2000.

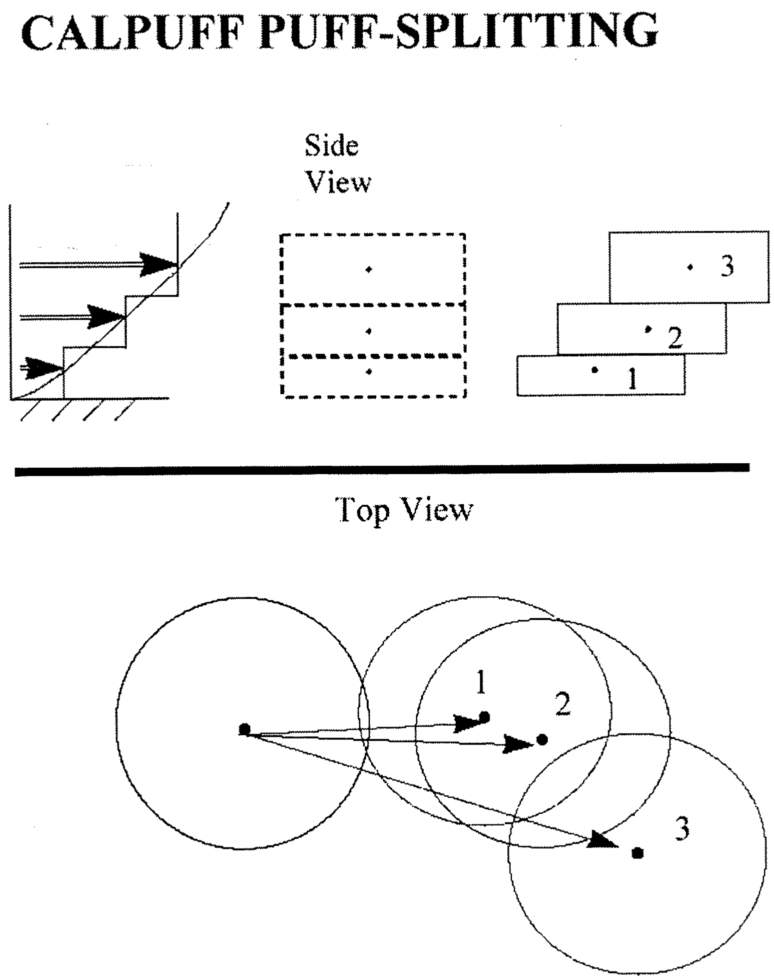
One aspect of mesoscale dispersion modeling that could help to explain the potential CALPUFF overpredictions involves vertical wind shear and its effects upon pollutant dispersion. In a paper delivered at the Eighth Joint Conference on Applications of Air Pollution Meteorology in 1994, Moran and Pielke discussed the importance of wind shear effects on enhancing, or even dominating, the horizontal dispersion during long-range transport. These authors showed with a numerical particle model that vertical shear of the horizontal flow could result in pollutants at different levels being advected at different speeds or in different directions. This situation is most likely to occur during the nighttime hours, when the vertical mixing in the atmosphere is often suppressed by stable thermal stratification. After the shape of a pollutant cloud becomes distorted by wind shear effects, subsequent or delayed vertical mixing will greatly enhance the horizontal spread of the cloud when it is mixed to the ground (see Figure 2-1). Moran and Pielke concluded that "the neglect of wind shear by mesoscale atmosphere dispersion models can result in significant errors in the prediction of tracer cloud size, shape, centroid location, and surface footprint if the cloud has experienced a sequence of at least two stability regimes." Note in Figure 2-1 that CALPUFF might tend to assume a plume spread as depicted in panels e or i while the actual plume spread after the morning inversion breakup is likely to better resemble panels h and l. Since CALPUFF may not have the capability to fully characterize the vertical shear effects, it is subject to the effect of underestimating the plume footprint, and overestimating the concentration.

Figure 2-1 Depiction of a pollutant cloud movement emitted during the CAPTEX experiment, showing the effects of delayed shear enhancement of the horizontal spreading of the cloud (from Moran and Pielke, 1994)



CALPUFF does have a puff splitting algorithm that is designed to respond to vertical wind shears across a puff. In effect, the algorithm causes puffs to be subdivided and the "daughter" puffs sent along different trajectories, leading to increased effective rate of puff dispersion and lower ground-level concentrations. There may be complex interactions between various parts of the CALPUFF modeling system and their cumulative effects upon this critically important puff splitting algorithm. For example, the way in which surface and upper level winds are weighted, extrapolated, and otherwise manipulated in CALMET can have a significant bearing on how effective the puff splitting algorithm works. In principle, the algorithm should split the puff into three parts and send these new puffs in different directions (see Figure 2-2), thereby effectively increasing the plume spread. However, the complex interactions between the construction of the wind field and the dispersion model may be such that seemingly unrelated processing decisions in CALMET (such as extrapolation of surface winds aloft, which could artificially reduce wind shear in the model) can significantly affect the dispersion results in CALPUFF, especially as they pertain to puff splitting. It is also evident from an inspection of the CALPUFF code that while the horizontal splitting in CALPUFF involves a computation of horizontal wind shear, this is not the case with the all-important vertical puff splitting. The vertical puff splitting tests merely check on the status of the puff elevation with respect to past and present mixing heights that the puff is or has experienced. Therefore, the full potential of vertical splitting may not be realized in CALPUFF, resulting in lost opportunities to respond to vertical wind shear.

Figure 2-2 Depiction of CALPUFF Handling of Puff Splitting (from CALPUFF User Manual, 1999)



The IWAQM Phase 2 report describes comparisons of CALPUFF predictions to tracer study observations in Section 4.6 of that report. The experiences encountered among the various experimental sites for CALPUFF can be summarized as follows:

- For individual events, the plume's trajectory missed the target by an angle on the order of 20 degrees, with considerable scatter.
- In a number of cases, the modeled plumes had higher central maximum concentrations and narrower dispersion than the observations indicated.
- Due to the relatively narrow plumes in CALPUFF, the directional error could mean significant changes in the predicted impacts. In some cases, this deficiency was countered by using a network of receptors rather than a single point prediction.

3.0 COMMENTS ON THE LIMITED CALPUFF EVALUATION

The EPA report relies upon a set of limited CALPUFF evaluations conducted by the NDDH to determine that the selection of technical options is appropriate. The most recent NDDH study used hourly emission rates from the major SO_2 sources and annual average emissions from the sources without hourly emissions data, such as the oil and gas sources. These emission inputs were paired with concurrent meteorological data for the year 2000. The CALPUFF predictions were compared to observations available at two SO_2 monitors located at Dunn Center and in the Theodore Roosevelt National Park, South Unit (unfortunately, the monitor in the TRNP North Unit was shut down in 1998). The locations of these monitors relative to the major SO_2 sources are shown in Figure 3-1. The resulting ranked concentrations unpaired in time but paired in space are shown in Figures 3-2 and 3-3 for Dunn Center (3-hour and 24-hour averages, respectively) and Figures 3-4 and 3-5 for TRNP, South Unit. The central diagonal line in each figure denotes a "perfect" model prediction for the line between the lower left and upper right corners. The other diagonal lines above and below the central diagonal line denote factor of two over prediction (the line above) and under prediction (the line below).

In general, the procedures used by the NDDH in their most recent study corrected deficiencies in the earlier study reported in 1999, which did not use hourly emission rates from the major sources. In addition, the emissions data in 2000 used a more accurate flow measurement technique that avoided overestimates of stack emissions associated with methods used prior to 2000.

The NDDH limited evaluation study conducted for the year 2000 can be further improved as noted below:

- Numerous oil and gas production sources beyond 50 kilometers from the monitors were not modeled. Their omission is accounted for in the estimate of regional background, discussed below.

- The monitors are both of the pulsed fluorescent type, with a threshold detection level of 2 parts per billion (ppb). Reported zero observed values were adjusted to half the threshold value (1 ppb) in the model evaluation study. However, zero predicted values were not similarly adjusted, leading to a potential underestimate of the predicted values.

- The EPA's Guideline on Air Quality Modeling (Appendix W of 40 CFR Part 51) states in Section 9.2 that the total predicted value should include a regional background value to account for natural background and unmodeled sources. In the evaluation study, the NDDH failed to follow this important step. In order to correct this omission, we have reviewed the evaluation procedures and the TRNP South Unit monitoring data for days with winds from a southerly direction, for which there are no upwind major SO_2 sources. We have also noted that the NDDH adjusted the observed zero values upward, but not the predicted zero values.

- The monitored values for days with southerly winds support a regional background value of at least 1 ppb. For the critical easterly wind cases with more population centers and more oil and gas sources, a regional background of 1.5 ppb (about 4 $\mu g/m^3$, and still below the instrument detection threshold) is reasonable. This value is still very low and is much lower than values typically used as regional background estimates in other rural states (e.g., the Alabama Department of Environmental Management (2000) uses a background concentration of 10 $\mu g/m^3$).

When a regional background of 4 $\mu g/m^3$ is added to the model predictions, the plots of the model evaluation results change significantly from the figures shown above, as seen in Figures 3-6 and 3-7 for the Dunn Center monitor and Figures 3-8 and 3-9 for the TRNP South Unit monitor. The EPA concern about model underpredictions is no longer valid (EPA's concerns were misplaced because the under prediction magnitude was at most only about 1 $\mu g/m^3$, well below the instrument threshold). The new results indicate that for Dunn Center (roughly 100 km from many of the major sources), CALPUFF over predicts on average by roughly 50% for the top several concentrations. For TRNP South Unit (roughly 150-200 km from many of the major sources), the CALPUFF over prediction tendency for the peak 3-hour concentrations is nearly 2.0, and it slightly exceeds 2.0 for the highest 24-hour averages.

These modified model evaluation results are consistent with the IWAQM Phase 2 report findings that warned of a CALPUFF model over prediction at the distances being considered for this modeling application. With corroboration from this limited evaluation study, the EPA modeling results are therefore likely to be subject to the same over prediction problem, and the findings from the EPA study must be viewed with these over prediction tendencies in mind. Either the EPA modeling procedures need to be corrected to eliminate the over prediction tendency, or the results need to be adjusted to account for the over prediction tendency.

Figure 3-1 **Map Showing Two SO_2 Monitoring Sites (Dunn Center and TRNP South Unit) and 12 Major SO_2 Sources. [1 = Coal Creek; 2 = Antelope Valley/Great Plain Synfuels; 3 = Coyote; 4 = Leland Olds/Stanton; 5 = Milton R Young; 6 = Heskett/Mandan Refinery ; 7 = Little Knife Gas; 8 = Grasslands Gas; 9 = Tioga Gas; 10 = Lignite Gas; 11 = Colstrip; 12 = CELP Boiler]**

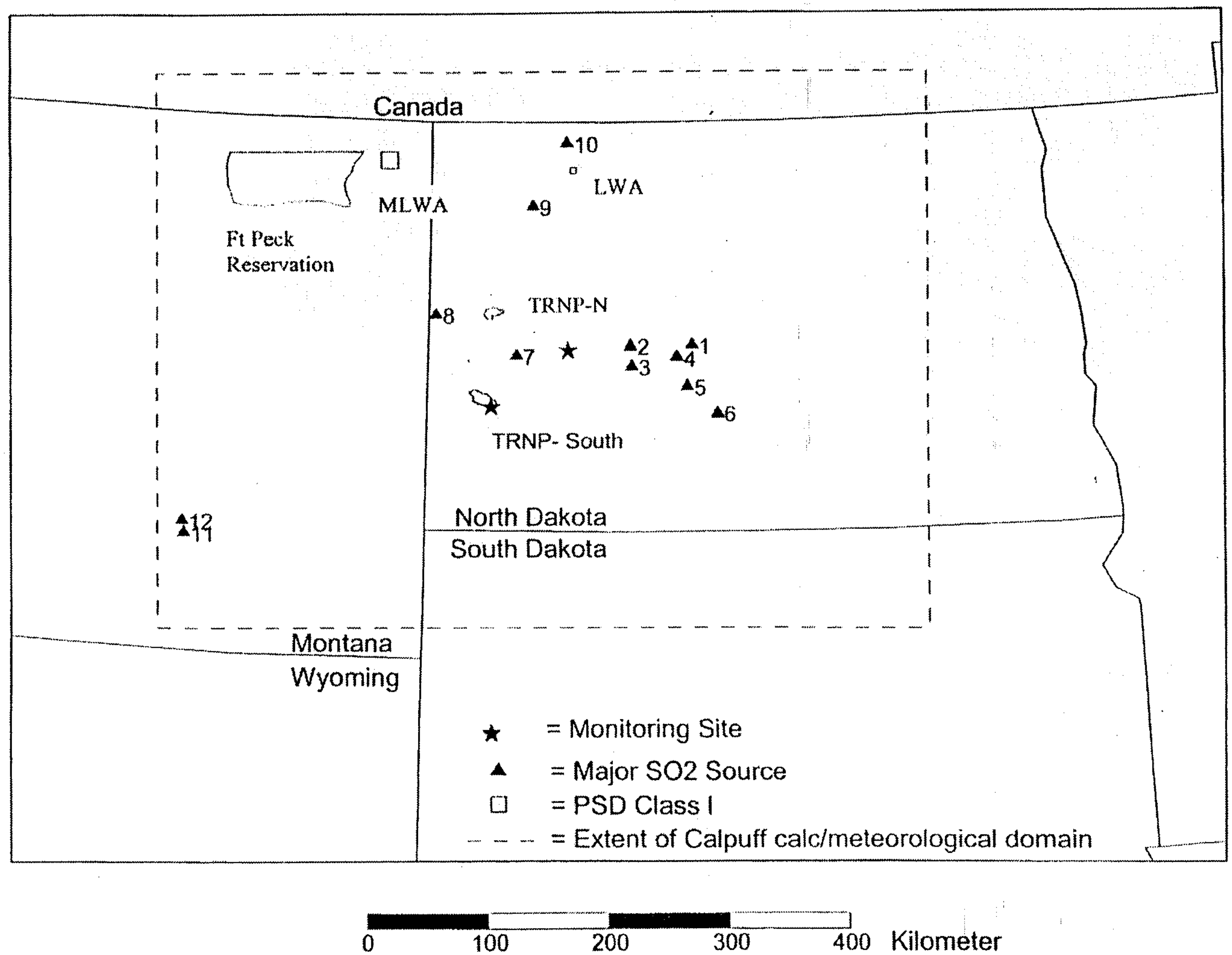


Figure 3-2 NDDH plot of CALPUFF Model Performance for Year 2000 (3-hour averages at Dunn Center)

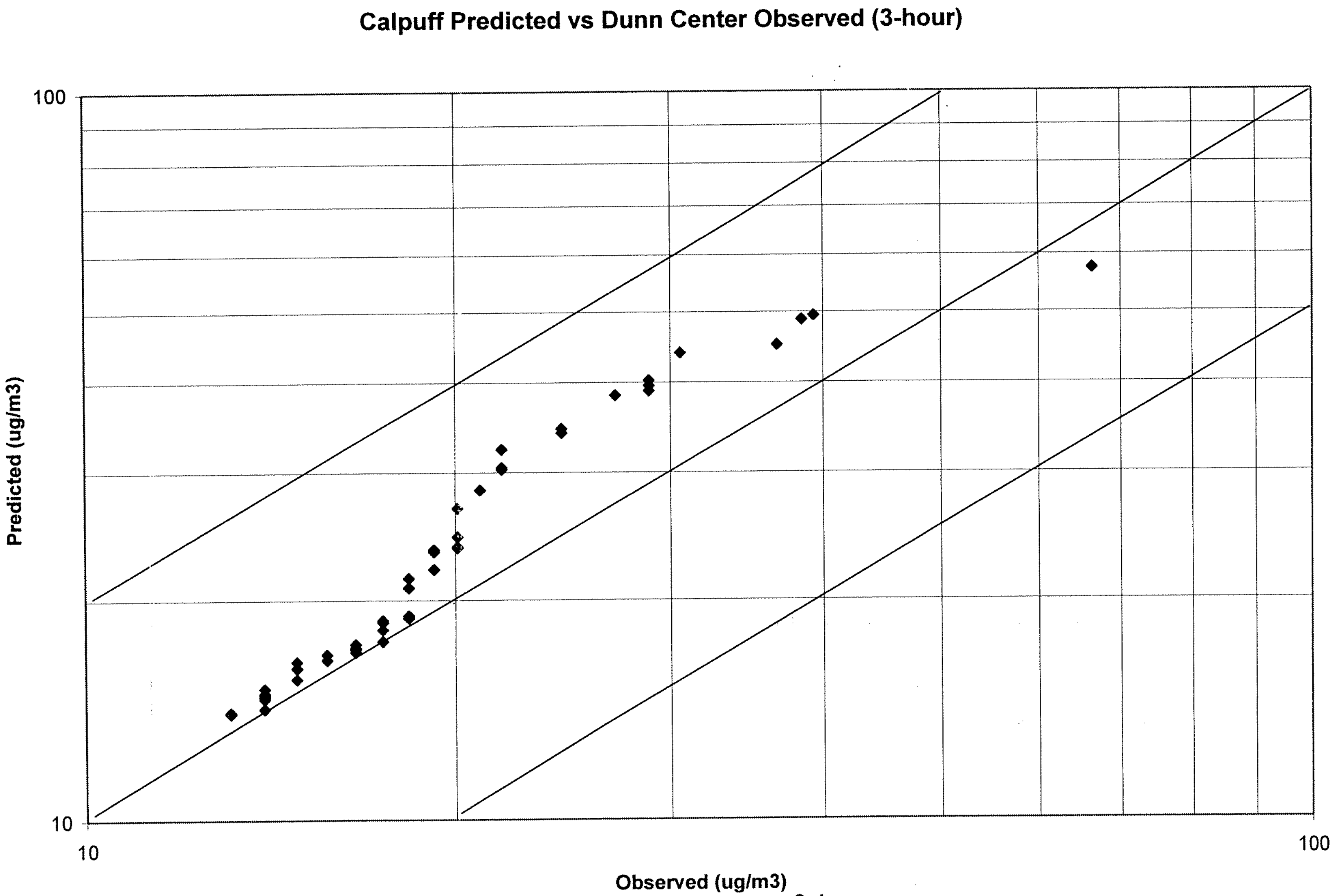


Figure 3-3 NDDH plot of CALPUFF Model Performance for Year 2000 (24-hour averages at Dunn Center)

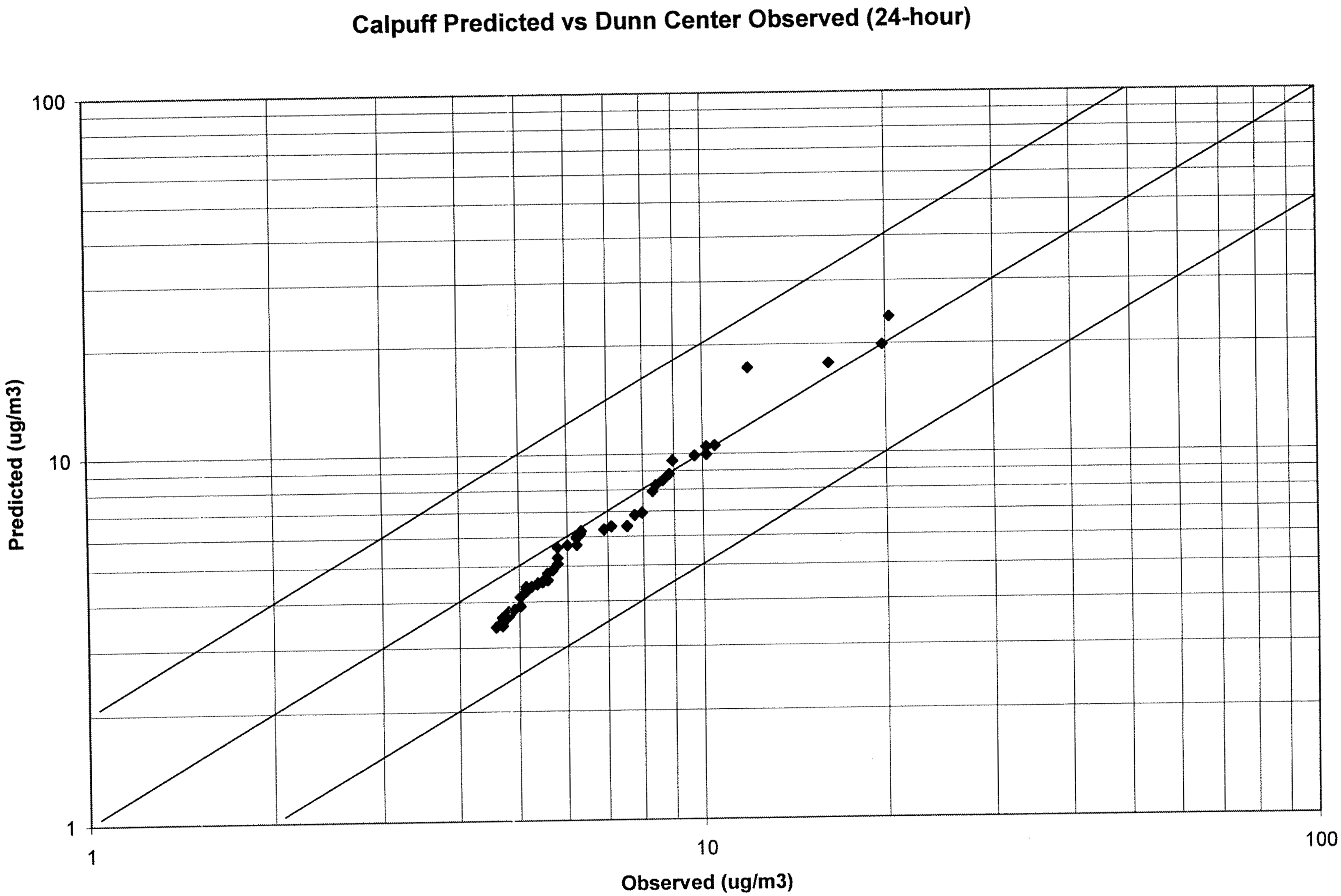


Figure 3-4 NDDH plot of CALPUFF Model Performance for Year 2000 (3-hour averages at TRNP South Unit)

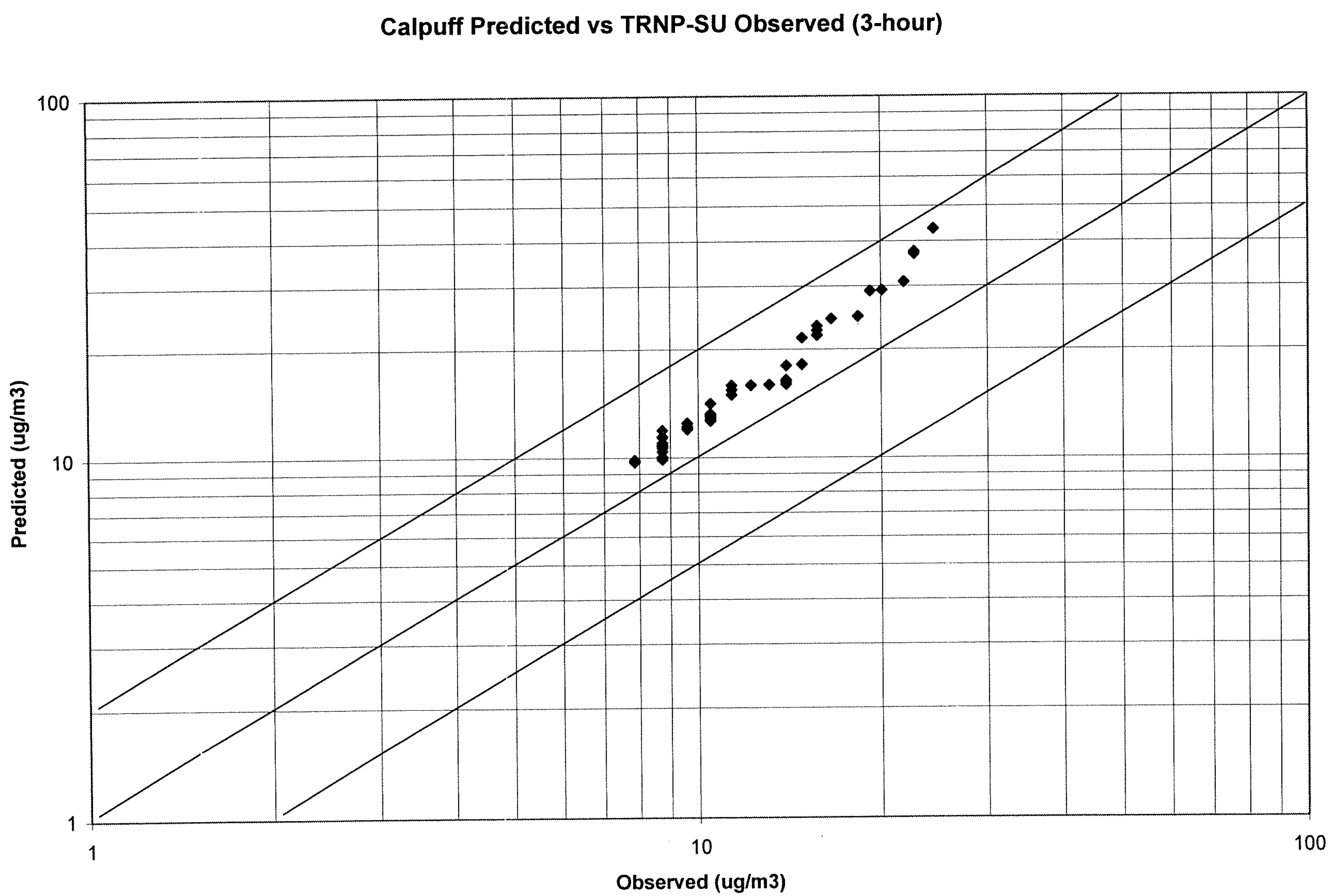


Figure 3-5 **NDDH plot of CALPUFF Model Performance for Year 2000 (24-hour averages at TRNP South Unit)**

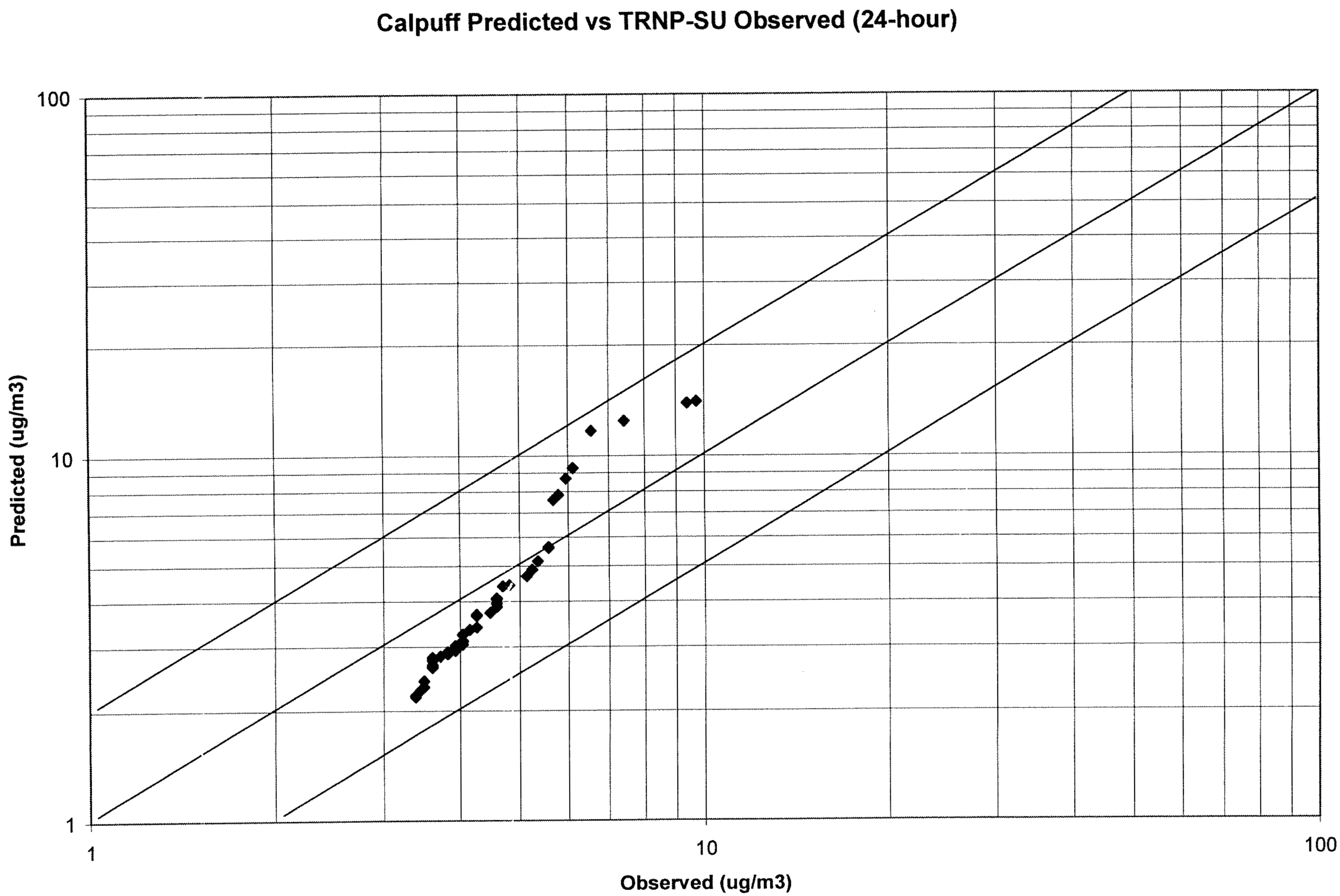


Figure 3-6 Modified plot of CALPUFF Model Performance for Year 2000 (3-hour averages at Dunn Center)

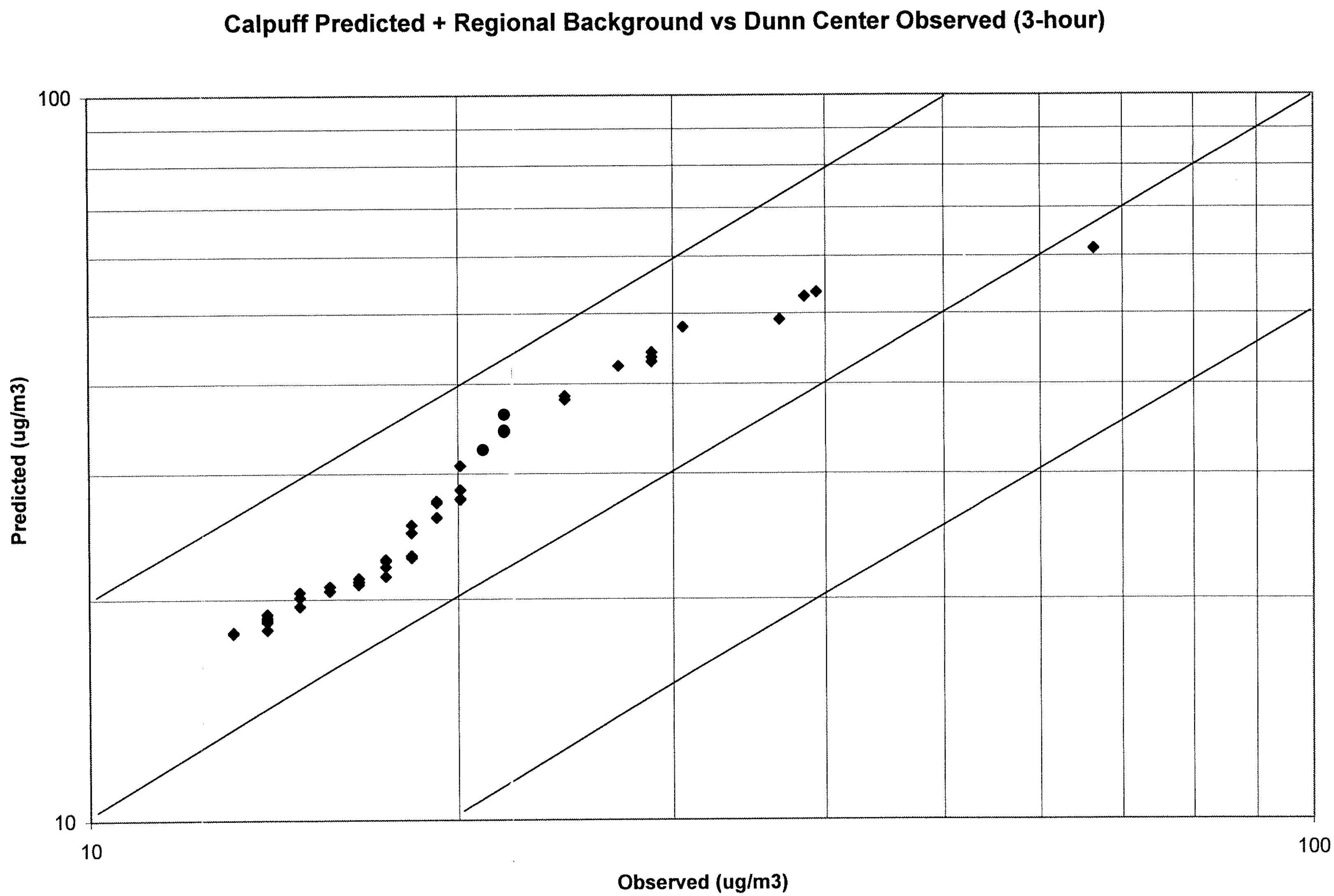


Figure 3-7 **Modified plot of CALPUFF Model Performance for Year 2000 (24-hour averages at Dunn Center)**

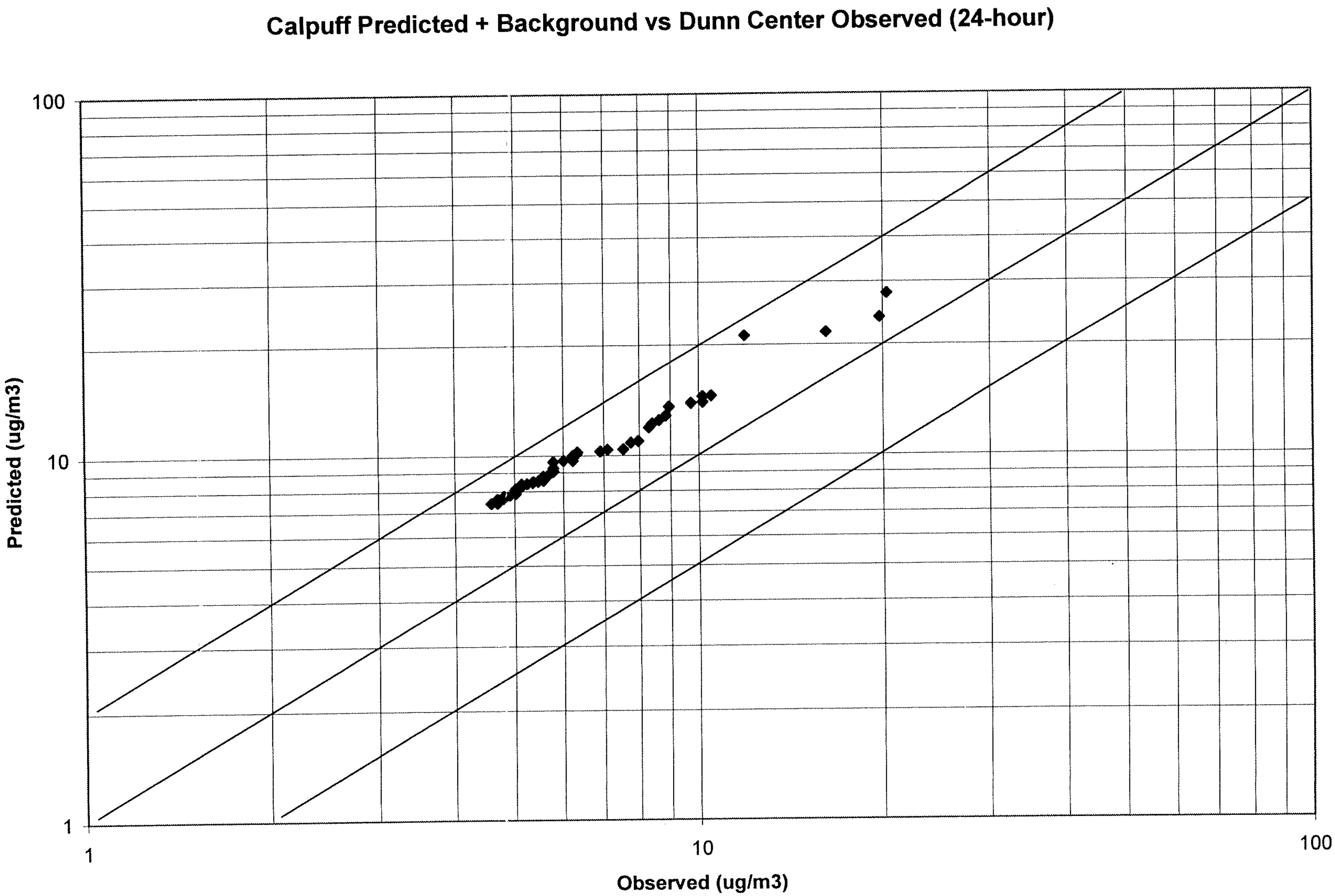


Figure 3-8 Modified plot of CALPUFF Model Performance for Year 2000 (3-hour averages at TRNP South Unit)

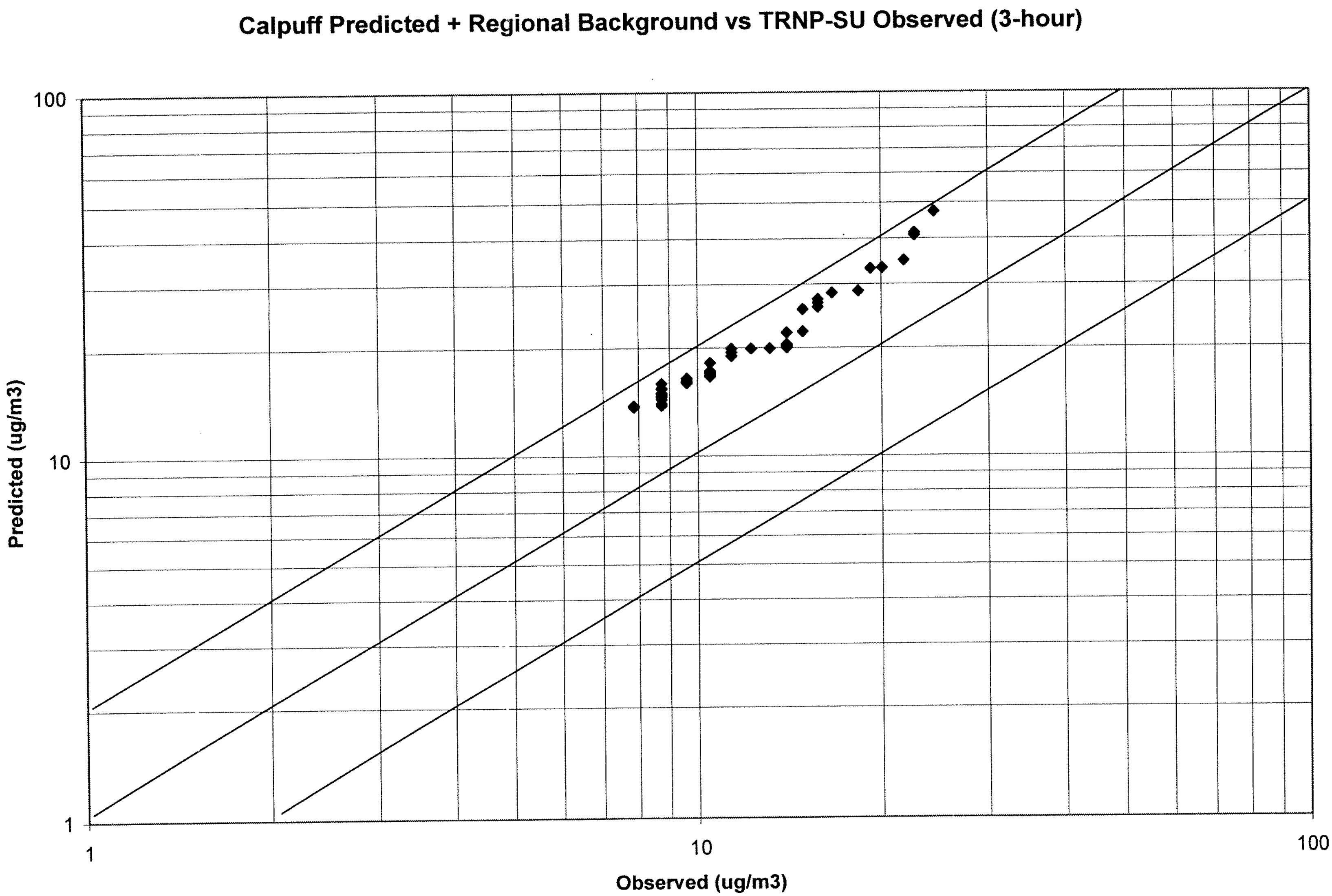


Figure 3-9 **Modified plot of CALPUFF Model Performance for Year 2000 (24-hour averages at TRNP South Unit)**